IgANets: Physics-Informed Machine Learning Embedded Into Isogeometric Analysis

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Aromath seminar

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Joint work with Deepesh Toshniwal, Frank van Ruiten (TUD),

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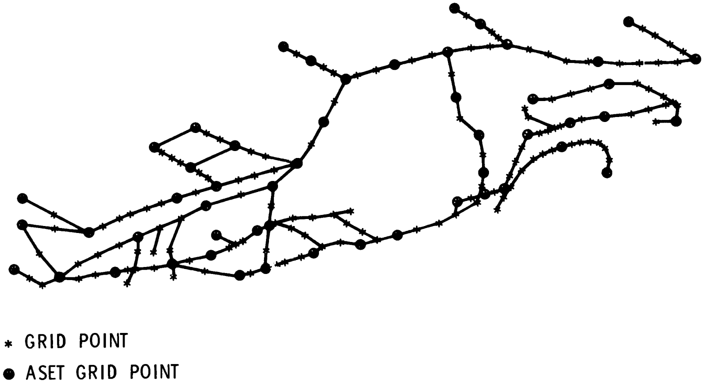
Design-through-Analysis

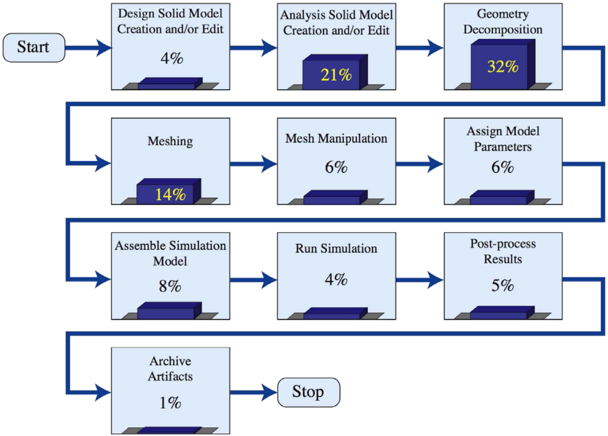
Design-through-Analysis 1.0

*"[...] the potential value of **design through analysis** was demonstrated by a significant reduction in structural weight of the project vehicle."*



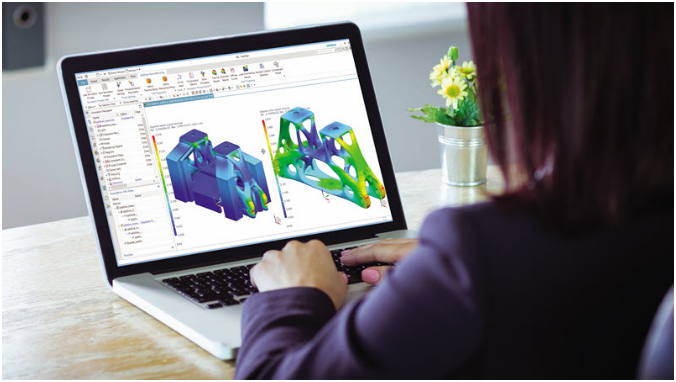
James A. Augustitus, Mounir M. Kamal, and Larry J. Howell. Design through analysis of an experimental automobile structure. SAE Transactions, 86:2186-2198, 1977

Design-through-Analysis 2.0



Vision: seamless design and analysis workflows without time-consuming (often manual) geometry cleaning and meshing → **Isogeometric Analysis** (Hughes et al. '05)

Interactive Design-through-Analysis

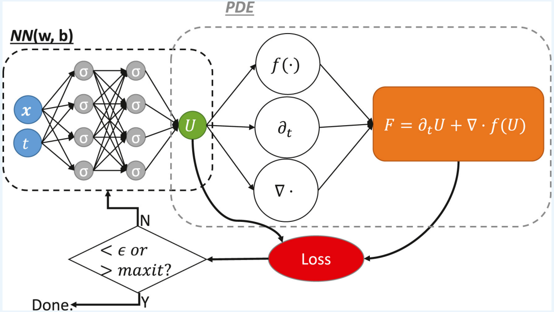


Vision: fast interactive qualitative analysis and accurate quantitative analysis within the same computational framework with seamless switching between both approaches

Photo: Siemens – Simulation for Design Engineers

Physics-informed machine learning

PINN (Raissi et al. 2018): *learns the (initial-)boundary-value problem*



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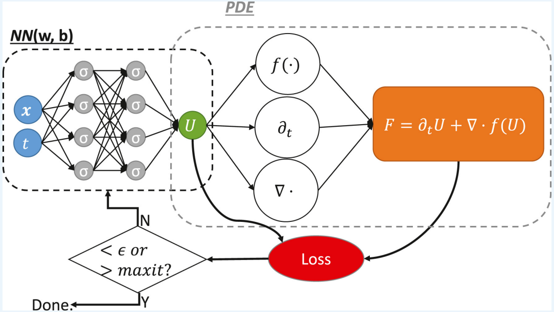

- easy to implement for ‘any‘ PDE because AD magic does it for you
- combined un-/supervised learning
- poor extrapolation/generalization
- point-based approach requires re-evaluation of NN at every point
- rudimentary convergence theory

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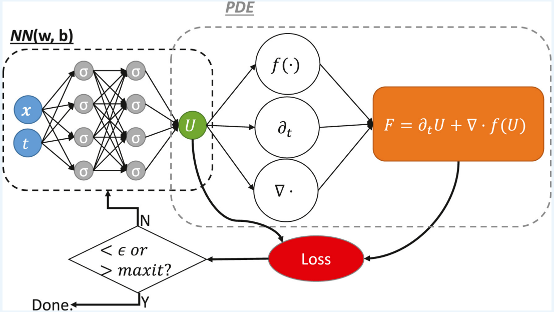

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$$G_\theta(u)(y) = \sum_{k=1}^{q} \underbrace{b_k(u(x_1), u(x_2), \ldots, u(x_m))}_{\text{branch}} \underbrace{t_k(y)}_{\text{trunk}}$$

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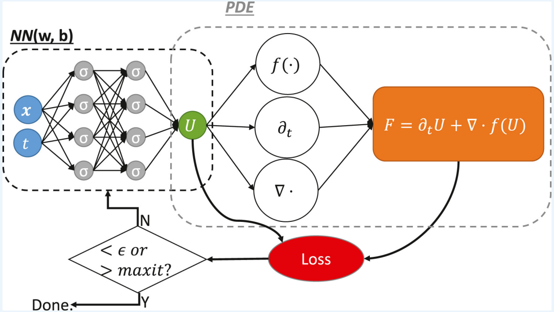

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Don't we know good bases?

Bases

AI/ML community: Fourier series, orthogonal polynomials, problem-specific basis functions $\rightarrow$ impractical for practical computer-aided geometric design

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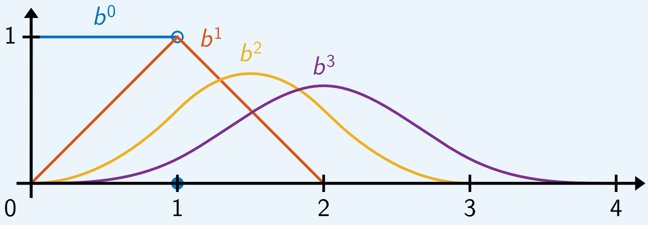
IGA community: multi-patch tensor-product or locally adaptive B-splines $\rightarrow$ Let's do it!

B-spline basis functions

Cox de Boor recursion formula



knot vector $\Xi = [0, 1, 2, 3, 4]$

$$b_i^0(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

$$b_i^p(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} b_i^{p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} b_{i+1}^{p-1}(\xi)$$

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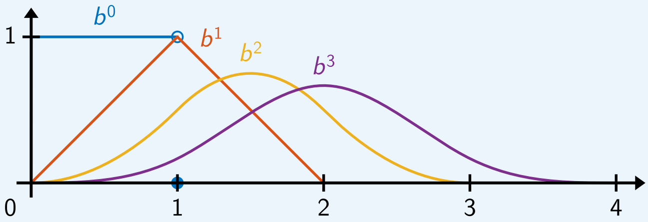

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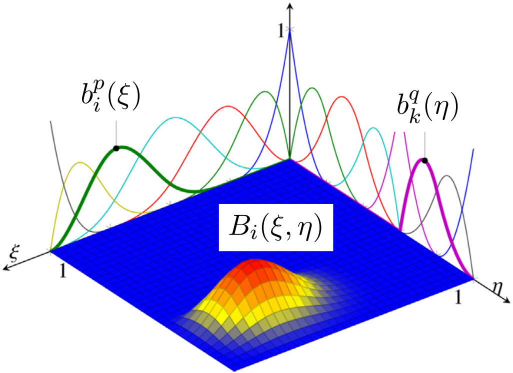
Many good properties: compact support $[\xi_i, \xi_{i+p+1})$, positive function values over support interval, derivatives of B-splines are combinations of lower-order B-splines, ...

Isogeometric Analysis

Paradigm: represent 'everything' in terms of tensor products of B-spline basis functions

$$B_i(\xi,\eta) := b_i^p(\xi)\cdot b_k^q(\eta), \qquad i := (k-1)\cdot n_i + i, \quad 1 \le i \le n_i, \quad 1 \le k \le n_k,$$



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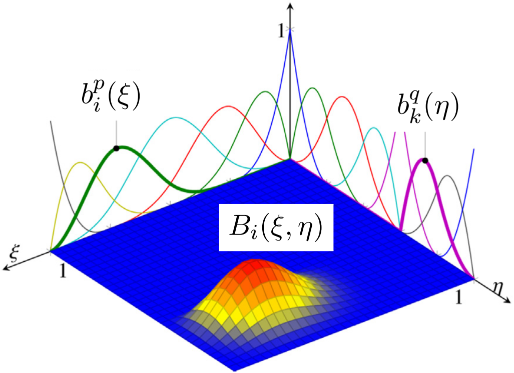
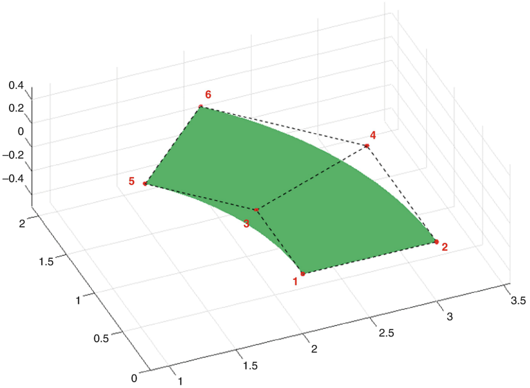


Many more good properties: partition of unity $\sum_{i=1}^{n} B_i(\xi,\eta) \equiv 1$, C^{p-1} continuity, ...

Isogeometric Analysis

Geometry: bijective mapping from the unit square to the physical domain $\Omega_h \subset \mathbb{R}^d$

$$\mathbf{x}_h(\xi, \eta) = \sum_{i=1}^{n} B_i(\xi, \eta) \cdot \mathbf{x}_i \qquad \forall (\xi, \eta) \in [0, 1]^2 =: \hat{\Omega}$$



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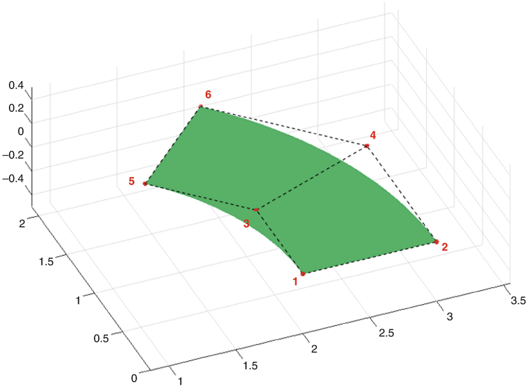

- the shape of Ω_h is fully specified by the set of **control points** $\mathbf{x}_i \in \mathbb{R}^d$
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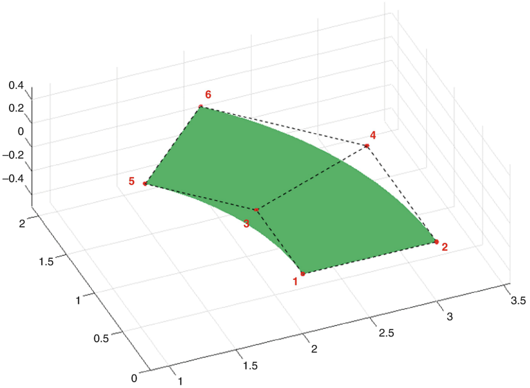

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- interior control points must be chosen such that 'grid lines' do not fold as this violates the bijectivity of $\mathbf{x}_h : \hat{\Omega} \rightarrow \Omega_h$
- refinement in h (knot insertion) and p (order elevation) preserves the shape of Ω_h and can be used to generate finer computational 'grids' for the analysis

Isogeometric Analysis

Model problem: Poisson's equation

$$-\Delta u_h = f_h \quad \text{in} \quad \Omega_h, \qquad u_h = g_h \quad \text{on} \quad \partial\Omega_h$$

with

$$\text{(geometry)} \qquad \mathbf{x}_h(\xi,\eta) = \sum_{i=1}^{n} B_i(\xi,\eta)\cdot \mathbf{x}_i \qquad \forall(\xi,\eta)\in[0,1]^2$$

$$\text{(solution)} \qquad u_h \circ \mathbf{x}_h(\xi,\eta) = \sum_{i=1}^{n} B_i(\xi,\eta)\cdot u_i \qquad \forall(\xi,\eta)\in[0,1]^2$$

$$\text{(r.h.s vector)} \qquad f_h \circ \mathbf{x}_h(\xi,\eta) = \sum_{i=1}^{n} B_i(\xi,\eta)\cdot f_i \qquad \forall(\xi,\eta)\in[0,1]^2$$

$$\text{(boundary conditions)} \qquad g_h \circ \mathbf{x}_h(\xi,\eta) = \sum_{i=1}^{n} B_i(\xi,\eta)\cdot g_i \qquad \forall(\xi,\eta)\in\partial[0,1]^2$$

Abstract representation

Given $\mathbf{x}_i$ (geometry), f_i (r.h.s. vector), and g_i (boundary conditions), **compute**

$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = A^{-1}\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}\right) \cdot b\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}\right)$$

Any point of the solution can afterwards be obtained by a simple **function evaluation**

$$(\xi,\eta) \in [0,1]^2 \quad \mapsto \quad u_h \circ \mathbf{x}_h(\xi,\eta) = [B_1(\xi,\eta),\ldots,B_n(\xi,\eta)] \cdot \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}$$

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Let us interpret the sets of B-spline coefficients $\{\mathbf{x}_i\}$, $\{f_i\}$, and $\{g_i\}$ as an efficient encoding of our PDE problem that is fed into our IgA machinery as **input**.

The **output** of our IgA machinery are the B-spline coefficients $\{u_i\}$ of the solution.

Isogeometric Analysis + Physics-Informed Machine Learning

IgANet: replace **computation**

$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = A^{-1}\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}\right) \cdot b\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}\right)$$

Isogeometric Analysis + Physics-Informed Machine Learning

IgANet: replace **computation** by **physics-informed machine learning**

$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = \text{IgANet}\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}; (\xi^{(k)}, \eta^{(k)})_{k=1}^{N_{\text{samples}}} \right)$$

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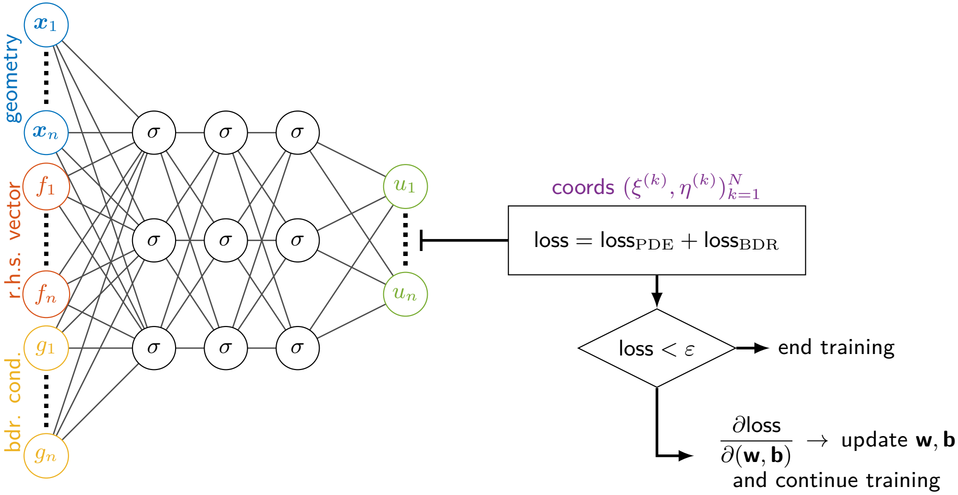
Compute the solution from the trained neural network as follows

$$u_h(\xi, \eta) = [B_1(\xi, \eta), \dots, B_n(\xi, \eta)] \cdot \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}, \quad \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = \text{IgANet}\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix} \right)$$

IgANet architecture



Loss function

Model problem: Poisson's equation with Dirichlet boundary conditions

$$\text{loss}_{\mathrm{PDE}} = \frac{\alpha}{N_\Omega} \sum_{k=1}^{N_\Omega} \left| \Delta \left[u_h \circ \mathbf{x}_h \left(\xi^{(k)}, \eta^{(k)} \right) \right] - f_h \circ \mathbf{x}_h \left(\xi^{(k)}, \eta^{(k)} \right) \right|^2$$

$$\text{loss}_{\mathrm{BDR}} = \frac{\beta}{N_\Gamma} \sum_{k=1}^{N_\Gamma} \left| u_h \circ \mathbf{x}_h \left(\xi^{(k)}, \eta^{(k)} \right) - g_h \circ \mathbf{x}_h \left(\xi^{(k)}, \eta^{(k)} \right) \right|^2$$

Express derivatives with respect to physical space variables using the Jacobian J, the Hessian H and the matrix of squared first derivatives Q (Schillinger *et al.* 2013):

$$\begin{bmatrix} \frac{\partial^2 B}{\partial x^2} \\ \frac{\partial^2 B}{\partial x \partial y} \\ \frac{\partial^2 B}{\partial y^2} \end{bmatrix} = Q^{-\top} \left(\begin{bmatrix} \frac{\partial^2 B}{\partial \xi^2} \\ \frac{\partial^2 B}{\partial \xi \partial \eta} \\ \frac{\partial^2 B}{\partial \eta^2} \end{bmatrix} - H^\top J^{-\top} \begin{bmatrix} \frac{\partial B}{\partial \xi} \\ \frac{\partial B}{\partial \eta} \end{bmatrix} \right)$$

Two-level training strategy

For $[\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathcal{S}_{\text{geo}}$, $[f_1, \dots, f_n] \in \mathcal{S}_{\text{rhs}}$, $[g_1, \dots, g_n] \in \mathcal{S}_{\text{bcond}}$ **do**

For a batch of randomly sampled $(\xi_k, \eta_k) \in [0,1]^2$ (or the Greville abscissae) **do**

$$\text{Train IgANet}\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}; (\xi_k, \eta_k)_{k=1}^{N_{\text{samples}}} \right) \mapsto \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}$$

EndFor

EndFor

Details:

- 7×7 bi-cubic tensor-product B-splines for $\mathbf{x}_h$ and u_h, C^2-continuous
- TensorFlow 2.6, 7-layer neural network with 50 neurons per layer and ReLU activation function (except for output layer), Adam optimizer, 30.000 epochs, training is stopped after 3.000 epochs w/o improvement of the loss value

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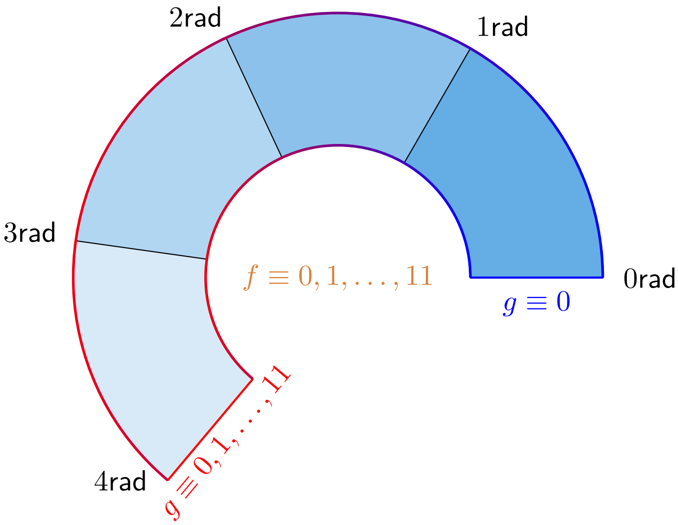
Test case: Poisson's equation on a variable annulus



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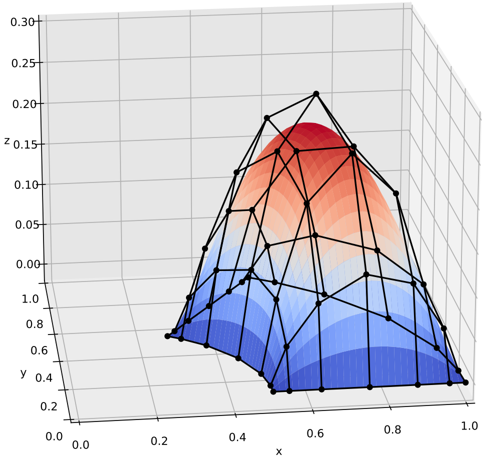
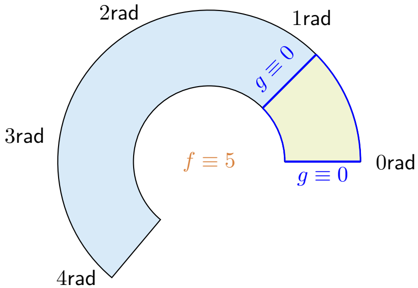
Preliminary results





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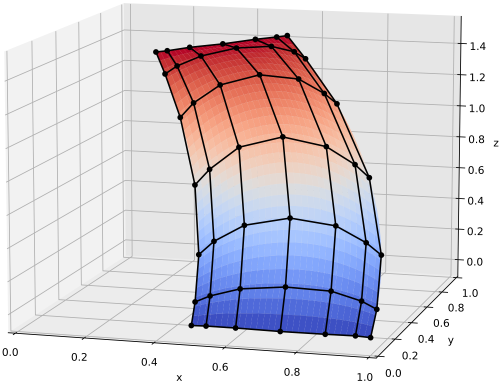

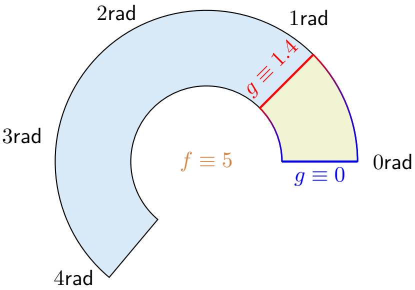

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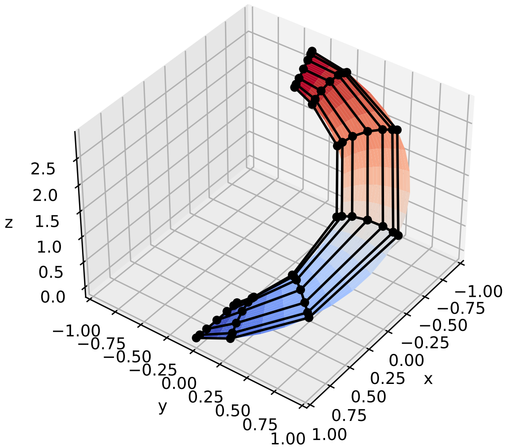

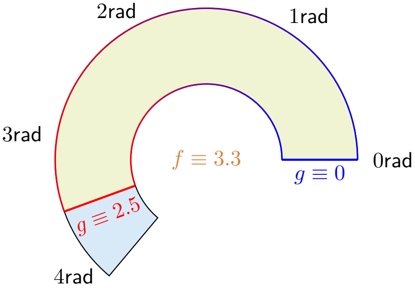

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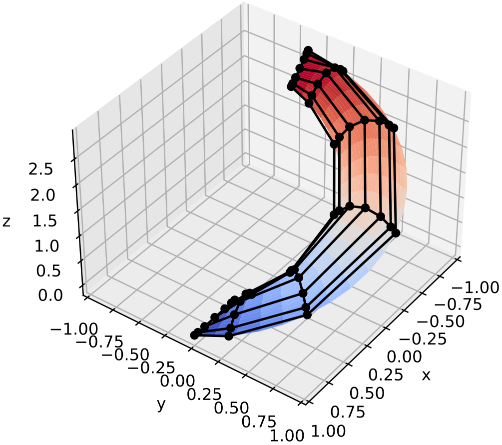

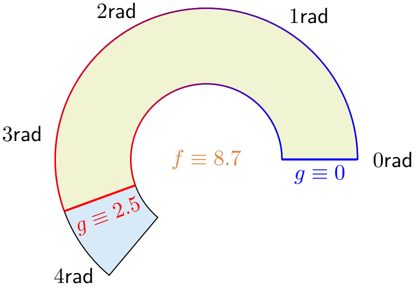

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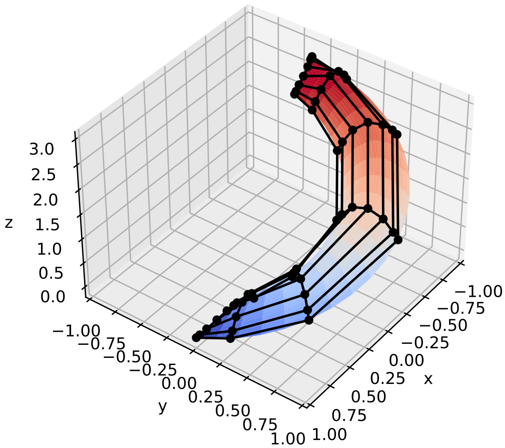

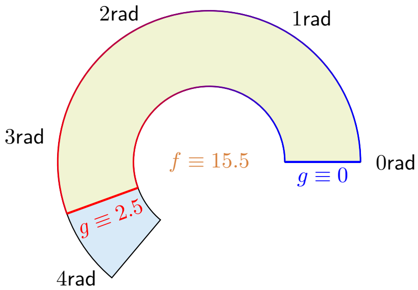

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Let's have a look under the hood

Computational costs of PINN vs. IgANets, implementation aspects, ...

Computational costs

Working principle of PINNs

$$\mathbf{x} \mapsto u(\mathbf{x}) := \mathsf{NN}(\mathbf{x}; f, g, G) = \sigma_L(\mathbf{W}_L\sigma(\ldots(\sigma_1(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1))) + \mathbf{b}_L)$$

- use AD engine (automated chain rule) to compute derivatives, e.g., $u_x = \mathsf{NN}_x$
- use AD engine on top of AD tree (!!!) to compute gradients w.r.t. weights for training

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Working principle of IgANets

$$[\mathbf{x}_i, f_i, g_i]_{i=1,\ldots,n} \mapsto [u_i]_{i=1,\ldots,n} := \mathsf{NN}(\mathbf{x}_i, f_i, g_i, i = 1, \ldots, n)$$

- use mathematics to compute derivatives, e.g., $\nabla_{\mathbf{x}} u = \left(\sum_{i=1}^n \nabla_{\boldsymbol{\xi}} B_i(\boldsymbol{\xi}) u_i\right) J_G^{-t}$
- use AD to compute gradients w.r.t. weights for training, i.e. (illustrated in 1D)

$$\frac{\partial(\mathrm{d}_\xi^r u(\xi))}{\partial w_k} = \sum_{i=1}^n \frac{\partial(\mathrm{d}_\xi^r b_i^p u_i)}{\partial w_k} = \cancel{\sum_{i=1}^n \mathrm{d}_\xi^{r+1} b_i^p \frac{\partial \xi}{\partial w_k} u_i} + \sum_{i=1}^n \mathrm{d}_\xi^r b_i^p \frac{\partial u_i}{\partial w_k}$$

Towards an ML-friendly B-spline evaluation

Major computational task (illustrated in 1D)

Given sampling point $\xi \in [\xi_i, \xi_{i+1})$ compute for $r \geq 0$

$$\mathrm{d}_\xi^r u(\xi) = \left[\mathrm{d}_\xi^r b_{i-p}^p(\xi), \ldots, \mathrm{d}_\xi^r b_i^p(\xi)\right] \cdot \underbrace{[u_{i-p}, \ldots, u_i]}_{\text{network's output}}$$

Textbook derivatives

$$\mathrm{d}_\xi^r b_i^p(\xi) = (p-1)\left(\frac{-\mathrm{d}_\xi^{r-1} b_{i+1}^{p-1}(\xi)}{\xi_{i+p} - \xi_{i+1}} + \frac{\mathrm{d}_\xi^{r-1} b_i^{p-1}(\xi)}{\xi_{i+p-1} - \xi_i}\right)$$

with

$$b_i^p(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} b_i^{p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} b_{i+1}^{p-1}(\xi), \quad b_i^0(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

Towards an ML-friendly B-spline evaluation

Matrix representation of B-splines (Lyche and Morken 2011)

$$\left[\mathrm{d}_\xi^r b_{i-p}^p(\xi), \ldots, \mathrm{d}_\xi^r b_i^p(\xi)\right] = \frac{p!}{(p-r)!} R_1(\xi) \cdots R_{p-r}(\xi) \mathrm{d}_\xi R_{p-r+1} \cdots \mathrm{d}_\xi R_p$$

with $k \times k+1$ matrices $R_k(\xi)$, e.g.

$$R_1(\xi) = \begin{bmatrix} \frac{\xi_{i+1}-\xi}{\xi_{i+1}-\xi_i} & \frac{\xi-\xi_i}{\xi_{i+1}-\xi_i} \end{bmatrix}$$

$$R_2(\xi) = \begin{bmatrix} \frac{\xi_{i+1}-\xi}{\xi_{i+1}-\xi_{i-1}} & \frac{\xi-\xi_{i-1}}{\xi_{i+1}-\xi_{i-1}} & 0 \\ 0 & \frac{\xi_{i+2}-\xi}{\xi_{i+2}-\xi_i} & \frac{\xi-\xi_i}{\xi_{i+2}-\xi_i} \end{bmatrix}$$

$$R_3(\xi) = \ldots$$

An ML-friendly B-spline evaluation

Algorithm 2.22 from (Lyche and Morken 2011)

1. $\mathbf{b} = 1$
2. For $k = 1, \dots, p - r$
    1. $\mathbf{t}_1 = (\xi_{i-k+1}, \dots, \xi_i)$
    2. $\mathbf{t}_2 = (\xi_{i+1}, \dots, \xi_{i+k})$
    3. $\mathbf{w} = (\xi - \mathbf{t}_1) \div (\mathbf{t}_2 - \mathbf{t}_1)$
    4. $\mathbf{b} = [(1 - \mathbf{w}) \odot \mathbf{b}, 0] + [0, \mathbf{w} \odot \mathbf{b}]$
3. For $k = p - r + 1, \dots, p$
    1. $\mathbf{t}_1 = (\xi_{i-k+1}, \dots, \xi_i)$
    2. $\mathbf{t}_2 = (\xi_{i+1}, \dots, \xi_{i+k})$
    3. $\mathbf{w} = 1 \div (\mathbf{t}_2 - \mathbf{t}_1)$
    4. $\mathbf{b} = [-\mathbf{w} \odot \mathbf{b}, 0] + [0, \mathbf{w} \odot \mathbf{b}]$

where $\div$ and $\odot$ denote the element-wise division and multiplication of vectors, respectively.

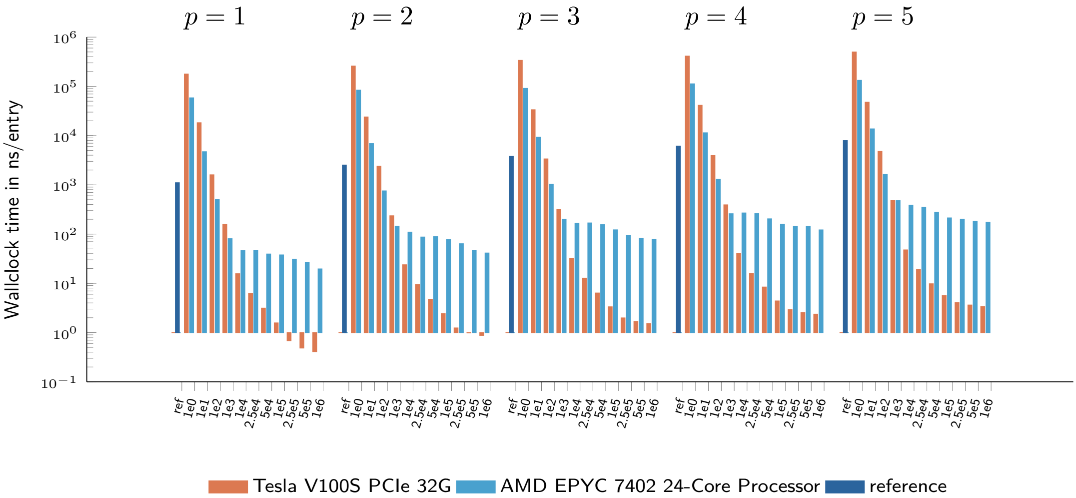
An ML-friendly B-spline evaluation

Algorithm 2.22 from (Lyche and Morken 2011) with slight modifications

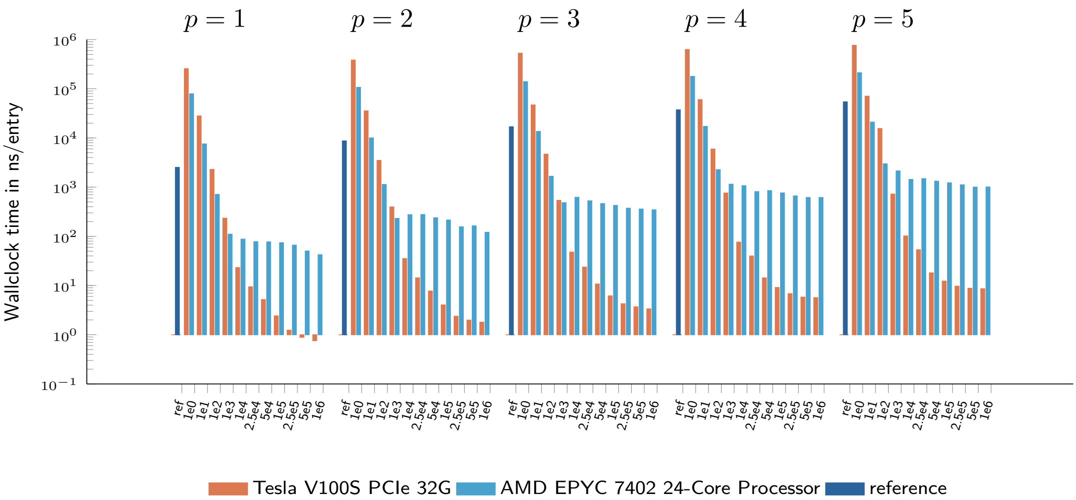
1. $\mathbf{b} = 1$
2. For $k = 1, \ldots, p - r$
    1. $\mathbf{t}_1 = (\xi_{i-k+1}, \ldots, \xi_i)$
    2. $\mathbf{t}_{21} = (\xi_{i+1}, \ldots, \xi_{i+k}) - \mathbf{t}_1$
    3. $\textbf{mask} = (\mathbf{t}_{21} < \text{tol})$
    4. $\mathbf{w} = (\xi - \mathbf{t}_1 - \textbf{mask}) \div (\mathbf{t}_{21} - \textbf{mask})$
    5. $\mathbf{b} = [(1 - \mathbf{w}) \odot \mathbf{b}, 0] + [0, \mathbf{w} \odot \mathbf{b}]$
3. For $k = p - r + 1, \ldots, p$
    1. $\mathbf{t}_1 = (\xi_{i-k+1}, \ldots, \xi_i)$
    2. $\mathbf{t}_{21} = (\xi_{i+1}, \ldots, \xi_{i+k}) - \mathbf{t}_1$
    3. $\textbf{mask} = (\mathbf{t}_{21} < \text{tol})$
    4. $\mathbf{w} = (1 - \textbf{mask}) \div (\mathbf{t}_{21} - \textbf{mask})$
    5. $\mathbf{b} = [-\mathbf{w} \odot \mathbf{b}, 0] + [0, \mathbf{w} \odot \mathbf{b}]$

where $\div$ and $\odot$ denote the element-wise division and multiplication of vectors, respectively.

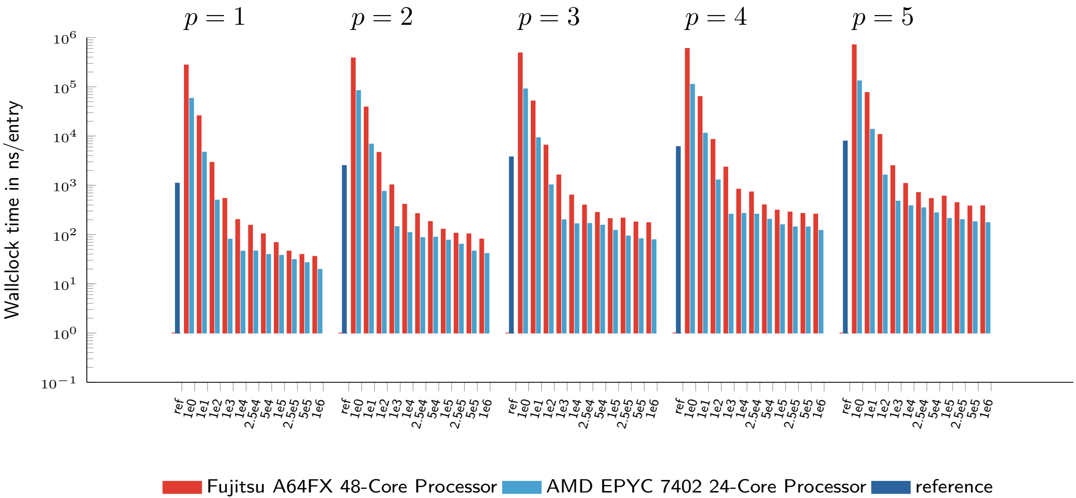
Performance evaluation - bivariate B-splines



Performance evaluation - trivariate B-splines

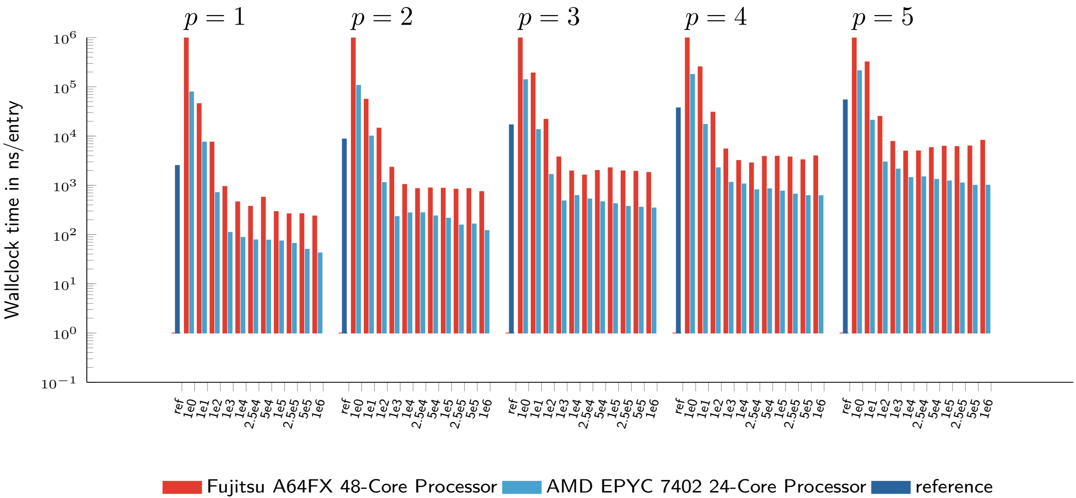


Performance evaluation - bivariate B-splines



Ookami Cluster @ Stony Brook: `gcc12.2 '-Ofast -mcpu=a64fx'`

Performance evaluation - trivariate B-splines



Ookami Cluster @ Stony Brook: `gcc12.2 '-Ofast -mcpu=a64fx'`

Interactive Design-through-Analysis

Front-ends

gustaf	Three.js modeler	???
by TU Vienna	by SURF	

WebSockets protocol for interactive spline modeling and visualization

Back-ends

	IgANet	???

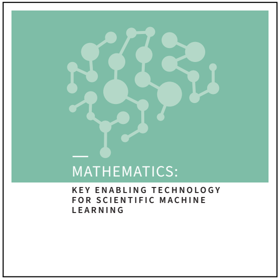
Conclusion and outlook

IgANets combine classical numerics with physics-informed machine learning and may finally enable **integrated and interactive design-through-analysis** workflows

WIP

- interactive DTA workflow (/w SURF)
- use of IgA and IgANets in concert
- transfer learning upon basis refinement

Short paper: Möller, Toshniwal, van Ruiten: *Physics-informed machine learning embedded into isogeometric analysis*, 2021. ☞



What's next

1. Journal paper and code release (including Python API) in preparation
2. CISM-ECCOMAS Summer School *Scientific Machine Learning in Design Optimization*

IgANets: Physics-Informed Machine Learning Embedded Into Isogeometric Analysis

Matthias Möller

Department of Applied Mathematics

Delft University of Technology, The Netherlands

Aromath seminar

25 April 2023, Sophia Antipolis Cedex, France

Joint work with Deepesh Toshniwal, Frank van Ruiten (TUD),

Casper van Leeuwen, Paul Melis (SURF), Jaewook Lee (TU Vienna)

Thank you very much!